

CLAIMS

What is claimed is:

1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
 - (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
 - (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
 - 5 (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
 - 10 (b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;
 - (c) outputting to said output device the constructed model.
3. A compound having a chemical structure selected using the method of claim 1,
15 said compound being an EPO mimetic.
4. The compound of claim 3 wherein said compound is not a peptide.
5. The compound of claim 3 wherein said compound is a peptide.
- 20 6. The compound of claims 5 wherein said peptide has 15 or fewer amino acids.